Snapshot Observation for 2D Classical Lattice Models by Corner Transfer Matrix Renormalization Group

Kouji Ueda, Ryota Otani, Yukinobu Nishio, Andrej Gendiar[2], and Tomotoshi Nishino

Department of Physics, Faculty of Science, Kobe University, Kobe 657-8501
[2] *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská cesta 9, SK-842 39 Bratislava, Slovakia*

(Received)

We report a way of obtaining a spin configuration snapshot, which is one of the representative spin configurations in canonical ensemble, in a finite area of infinite size two-dimensional (2D) classical lattice models. The corner transfer matrix renormalization group (CTMRG), a variant of the density matrix renormalization group (DMRG), is used for the numerical calculation. The matrix product structure of the variational state in CTMRG makes it possible to stochastically fix spins each by each according to the conditional probability with respect to its environment.

§1. Introduction

For a classical lattice spin system that interacts with a reservoir, the spin configuration observed at an instant, which we call *snapshot* in the following, is one of the representative configurations in the canonical ensemble. Such a snapshot is experimentally observed if the time scale of the observation is much shorter than that of the evolution of the system. A *freezed* spin configuration after sudden cooling can also be regarded as a kind of snapshot. In general, snapshots show rough outlook of the system. For example, the typical size of a spin inverted island in the ordered state is of the order of the correlation length, and symmetries of ordered states can be intuitively identified. Figure 1 shows a snapshot inside the area of 100 by 100 of the two-dimensional (2D) ferromagnetic Ising model, where the system size is much larger than the shown region. Normally such a snapshot is drawn by Monte Carlo simulation,[1] while the shown one is created by the corner transfer matrix renormalization group[7] (CTMRG), a variant of the density matrix renormalization group[2] (DMRG) applied to 2D classical lattice models. So far both DMRG and CTMRG have been used for calculations of thermal average of spin correlation functions, but not for the snapshots.

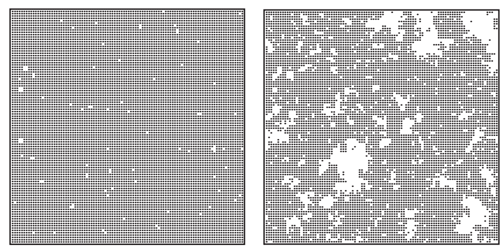

Fig. 1. Snapshots of the ferromagnetic Ising model at $T = 1.5$ (left) and 2.27 (right), where we have chosen the nearest neighbor coupling constant as the unit of energy.

In this article we report a way of obtaining the conditional probability for a row of spins of length N surrounded by the rest of the system, using the matrix product structure[3] (MPS) of the variational state employed in CTMRG and DMRG. These spins can be fixed one by one according to the conditional probability, and after fixing all the spins in the row it is possible to obtain the conditional probability for the next row in the same manner. Applying such a fixing process for M numbers of rows, one obtains a snapshot for the area of N by M in infinite — or sufficiently large — 2D lattice systems. Numerical cost for this snapshot observation is of the same order of conventional zipping process in the finite system DMRG algorithm.[2,4]

In the next section we briefly explain how to fix a spin in the 2D lattice model in terms of the corner transfer matrix formalism. In section 3 we generalize the spin fixing procedure to a row of spins of the length N, by taking partial sum for the inner product between MPSs. Introducing position dependence to the local factors that construct MPS, we successively fix the M-rows of spins as we explain in Sec.4. In the last section we conclude the result and discuss the relation with quantum observation in one dimension.

§2. One Spin Fixing

The corner transfer matrix (CTM), which was invented by Baxter,[5] is not only useful for rigorous analyses of 2D lattice systems, but also efficient for numerical calculations of thermodynamic functions, especially away from the critical point. Let us briefly look at the construction of CTM and the block spin transformation applied for it.

We consider the square lattice Ising model as an example of the 2D classical lattice spin models. The partition function of the system is expressed as

$$Z = \sum_{\{\sigma\}} \exp(H\{\sigma\}) \, , \tag{2.1}$$

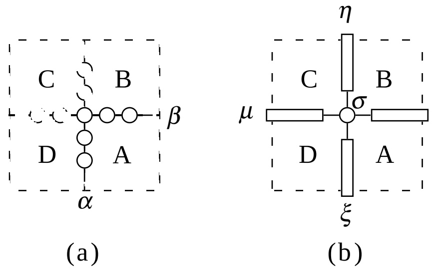

Fig. 2. Division of the 2D lattice into 4 corners. (a) Variables of the corner transfer matrix A. (b) Renormalized corner transfer matrices.

where $\{\sigma\}$ represents a configuration of Ising spins $\sigma = \pm 1$ on the square lattice, and $H\{\sigma\}$ is the Ising Hamiltonian, that is a sum of Ising interaction over all the bonds.

In the CTM formalism, the 2D lattice is divided into 4 parts, so called the quadrants or the corners.[5)] Let us label each quadrant as A, B, C, and D. The Hamiltonian $H\{\sigma\}$ is then expressed as sum of the corresponding parts

$$H_A\{\sigma_A\} + H_B\{\sigma_B\} + H_C\{\sigma_C\} + H_D\{\sigma_D\}\,, \qquad (2.2)$$

where $\{\sigma_A\}$, $\{\sigma_B\}$, $\{\sigma_C\}$, and $\{\sigma_D\}$ denote spin configurations in each quadrant of the system. Note that neighboring quadrants share the same spins at the boundary between them. In this way the Boltzmann weight of the whole system is expressed as a product of 4 factors

$$\begin{aligned}\exp(H\{\sigma\}) = & \exp(H_A\{\sigma_A\})\exp(H_B\{\sigma_B\}) \\ & \exp(H_C\{\sigma_C\})\exp(H_D\{\sigma_D\})\,. \qquad (2.3)\end{aligned}$$

The corner transfer matrix is the partial sum of each factor with respect to the spins *inside* the corner

$$A(\alpha\sigma\beta) = {\sum_{\{\sigma_A\}}}' \exp(H_A\{\sigma_A\}) \qquad (2.4)$$

except for those spins at the boundary with other corners, where the notation $\sum'$ denotes this restricted summation, and where α and β denotes groups of spins at the boundary. (See Fig. 2 (a).) The CTM is a block diagonal matrix with respect to σ, while in this article we do not use this matrix property explicitly. Other CTMs B, C, and D are defined in the same manner. If the system is invariant under the rotation of 90 degree these CTMs are equivalent. For simplicity, we assume this symmetry in the following.

The matrix dimension of the CTM increases exponentially with the system size. In order to avoid this blow up and treat the CTM accurately in numerical calculation, block spin transformation is introduced in CTMRG from those spins α and β at the boundary to m-state auxiliary variables. Such a transformation maps the CTM A into the compressed (or renormalized) one

$$A(\xi\sigma\nu) = \sum_{\alpha\beta} U_\xi(\alpha)\, U_\nu(\beta)\, A(\alpha\sigma\beta)\;, \qquad (2.5)$$

where ξ and ν are the m-state auxiliary variables. The transformation matrix $U_\xi(\alpha)$ is obtained by diagonalizing the density matrix $\rho = ABCD$.[2,6)] Other CTMs can also be mapped to $B(\nu\sigma\eta)$, $C(\eta\sigma\mu)$, and $D(\mu\sigma\xi)$ as shown in Fig. 2 (b). The approximate partition function

$$Z' = \sum_{\sigma}\sum_{\xi\nu\eta\mu} A(\xi\sigma\nu)\, B(\nu\sigma\eta)\, C(\eta\sigma\mu)\, D(\mu\sigma\xi) \qquad (2.6)$$

is close enough to the original one Z in Eq. (2.1) if m is sufficiently large; normally m is of the order of 10 to 1000.

When the system size is far larger than the correlation length of the system, the renormalized CTMs becomes independent of the system size except for a constant multiple. Throughout this article we assume such a condition, and regard the renormalized CTM as a quadrant of *infinite* size systems.

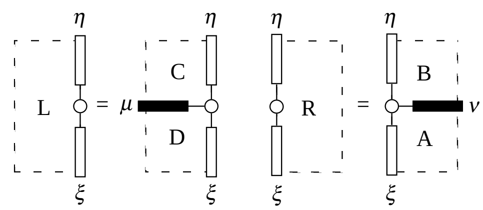

Fig. 3. The left and the right vectors created from CTMs.

Now we calculate the probability of observing $\sigma = 1$ (up) and $\sigma = -1$ (down) at the center of the system. We first prepare two partial sums

$$L(\eta\sigma\xi) = \sum_{\mu} C(\eta\sigma\mu)\, D(\mu\sigma\xi)$$

$$R(\xi\sigma\eta) = \sum_{\nu} A(\xi\sigma\nu)\, B(\nu\sigma\eta)\,, \qquad (2.7)$$

that we regard $2m^2$-dimensional vectors in the following. Figure 3 shows the graphical representation of the above equation. The order of variables in $L(\eta\sigma\xi)$ is opposite to that of $R(\xi\sigma\eta)$, since we keep the order of auxiliary variables in the right hand sides of the above equations. The approximate partition function Z' is represented as

$$Z' = \langle L|R\rangle \equiv \sum_{\xi\sigma\eta} L(\eta\sigma\xi)\, R(\xi\sigma\eta)\,, \qquad (2.8)$$

where we have introduced bracket notations for the book keeping. The probability of σ taking the specific value $\bar\sigma$ can be written as

$$p(\bar\sigma) = \frac{\langle L|\,\delta(\bar\sigma,\sigma)\,|R\rangle}{\langle L|R\rangle} = \frac{\sum_{\xi\eta} L(\eta\bar\sigma\xi)\, R(\xi\bar\sigma\eta)}{\sum_{\xi\sigma\eta} L(\eta\sigma\xi)\, R(\xi\sigma\eta)}\,, \qquad (2.9)$$

where the probability satisfies the normalization $p(1) + p(-1) = 1$. Therefore, creating a random number x in the range $[0, 1)$ one can fix σ to $\bar\sigma = 1$ if $x < p(1)$, otherwise to $\bar\sigma = -1$.

§3. Snapshot in a row

Let us generalize the spin fixing procedure to a N numbers of spins in a row from σ_1 to σ_N, where N is much smaller than the system size. For this purpose we introduce the half-row transfer matrices (HRTMs), that are upper and lower halves of the transfer matrix T to the horizontal direction. Figure 4 shows the system that we consider in this section. Between the vectors L and R, there are $N-1$ numbers of transfer matrix

$$T_i = S_i P_i \tag{3.1}$$

from $i = 1$ to $N-1$, where S_i and P_i are HRTMs

$$\begin{aligned} S_i &= S(\xi_i\, \sigma_i\, \sigma_{i+1}\, \xi_{i+1}) \\ P_i &= P(\eta_{i+1}\, \sigma_{i+1}\, \sigma_i\, \eta_i)\,. \end{aligned} \tag{3.2}$$

We have aligned the variables of HRTMs in the clockwise order as CTMs. At the moment all the HRTMs are equivalent, though we put indices for identification of their positions.

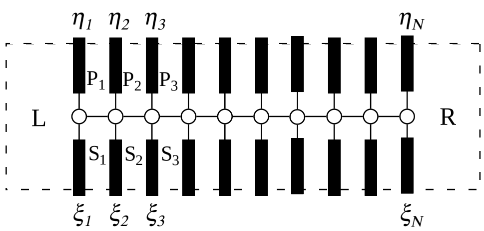

Fig. 4. Half-row transfer matrices between vectors L and R.

We fix these N spins from the left to the right, successively calculating the conditional probability $p_{\bar{\sigma}_1 \ldots \bar{\sigma}_{i-1}}(\bar{\sigma}_i)$ for the spin at i-site after fixing those spins in the left $\bar{\sigma}_1, \ldots, \bar{\sigma}_{i-1}$. The way of calculation is essentially the same as operator multiplication to a given matrix product state[3–5] (MPS) in finite system DMRG algorithm, and it is numerically important to prepare partial sum of local factors in advance. We write R as R_N since it contains σ_N as its variable. Let us multiply the transfer matrices T_i one by one to the vector R_N. We obtain

$$\begin{aligned} R_{N-1} &= T_{N-1}\, R_N \\ R_{N-2} &= T_{N-2}\, R_{N-1}\,, \ \text{etc.,} \end{aligned} \tag{3.3}$$

down to R_1. In the numerical calculation we do not possess the transfer matrix T_i explicitly, but we apply S_i and P_i part by part as

$$R(\eta_i \sigma_i \xi_i) = \sum_{\sigma_{i+1}\xi_{i+1}} S(\xi_i \sigma_i \sigma_{i+1} \xi_{i+1}) \sum_{\eta_{i+1}} R(\xi_{i+1}\sigma_{i+1}\eta_{i+1}) P(\eta_{i+1}\sigma_{i+1}\sigma_i \eta_i)\,, \tag{3.4}$$

where the second sum should be taken first. (See Fig. 5.)

After obtaining R_1 we can calculate the probability for

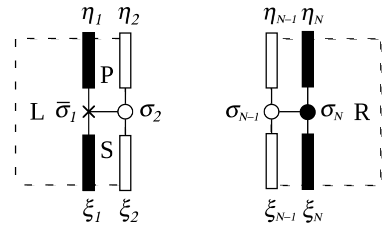

Fig. 5. Multiplication of Transfer Matrix.

σ_1 as before

$$p(\bar{\sigma}_1) = \frac{\langle L_1 |\, \delta(\bar{\sigma}_1, \sigma_1)\, | R_1 \rangle}{\langle L_1 | R_1 \rangle}\,, \tag{3.5}$$

where we have written L as L_1 since it contains σ_1 as its variable. According to this probability we stochastically fix the first spin in the row. We then consider the conditional probability $p_{\bar{\sigma}_1}(\bar{\sigma}_2)$ for the second spin after fixing the first one. This time, we have to prepare L_1 multiplied by T

$$L(\eta_2\sigma_2\xi_2) = \sum_{\eta_1} P(\eta_2\sigma_2\bar{\sigma}_1\eta_1) \sum_{\xi_1} L(\eta_1\bar{\sigma}_1\xi_1) S(\xi_1\bar{\sigma}_1\sigma_2\xi_2) \tag{3.6}$$

as shown in Fig. 5. It should be noted that we *do not* take configuration sum for $\bar{\sigma}_1$ since it is already fixed; L_2 contains a fixed spin $\bar{\sigma}_1$ in it. Using R_2 calculated before and L_2 in Eq.(3.6), we obtain the conditional probability for the second spin

$$p_{\bar{\sigma}_1}(\bar{\sigma}_2) = \frac{\langle L_2 |\, \delta(\bar{\sigma}_2, \sigma_2)\, | R_2 \rangle}{\langle L_2 | R_2 \rangle}\,. \tag{3.7}$$

According to this probability we can fix the second spin. After that we calculate L_3 in the same manner as Eq.(3.6). Repeating these spin fixing procedure to σ_N, we finally obtain a spin snapshot $\{\bar{\sigma}\} = \bar{\sigma}_1, \bar{\sigma}_2, \ldots, \bar{\sigma}_N$ for a group of N spins in a row.

§4. Snapshot in a Rectangular Area

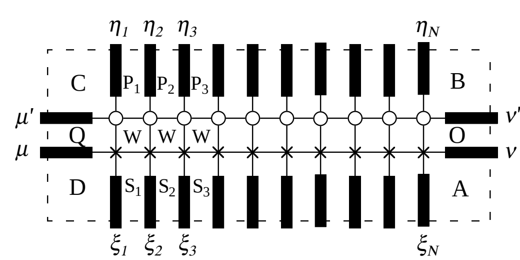

Fig. 6. The double-row spin system. The cross marks represent the already fixed spins in the first row, and the circles are those spins that we will fix each by each.

Let us consider the way of fixing M numbers of spin rows successively. The first step is to obtain the probability for the second spin row under the condition that the first row $\bar{\sigma}_1, \bar{\sigma}_2, \ldots, \bar{\sigma}_N$ is already fixed. For the distinction let us write the spins in the second row as $\{\tau\} =$

$\tau_1, \tau_2, \ldots, \tau_N$. Figure 6 shows the system that we consider for a while, where there is a transfer matrix to the vertical direction between $\{\bar{\sigma}\}$ shown by cross marks and $\{\tau\}$ by circles. This transfer matrix consists of the right HRTM $O(\nu\bar{\sigma}_N\tau_N\nu')$, the left one $Q(\mu'\tau_1\bar{\sigma}_1\mu)$, and $N-1$ numbers of local Boltzmann weights $W(\tau_i\,\tau_{i+1}\bar{\sigma}_i\,\bar{\sigma}_{i+1}\ )$ from $i=1$ to $N-1$ in between.[8]

We reduce the above double-row system to the single-row one treated in the previous section by way of extension of the CTMs and HRTMs to the vertical direction, similar to the system size extension in CTMRG.[7] The HRTM S is extended by putting W on top of it

$$S'(\xi_i\,\tau_i\,\tau_{i+1}\xi_{i+1}) = W(\tau_i\,\tau_{i+1}\bar{\sigma}_i\,\bar{\sigma}_{i+1}\ )S(\xi_i\,\bar{\sigma}_i\,\bar{\sigma}_{i+1}\xi_{i+1}) \tag{4.1}$$

as shown in Fig. 7. Here we do not regard $\bar{\sigma}_i$ and $\bar{\sigma}_{i+1}$ as the variable of the extended HRTM S' since these are *fixed constants*. Thus the number of elements in S'_i is the same as that of S_i. It should be noted that after such an extension S'_i becomes position dependent.

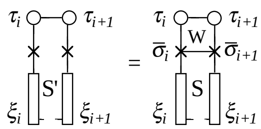

Fig. 7. Extension of the HRTM S to the vertical direction.

The area extension of CTMs A and D are done by putting HRTMs O and Q

$$A'(\xi_N\tau_N\nu') = \sum_{\nu} A(\xi_N\bar{\sigma}_N\nu)\,O(\nu\bar{\sigma}_N\tau_N\nu')$$

$$D'(\mu'\tau_1\xi_1) = \sum_{\mu} Q(\mu'\tau_1\bar{\sigma}_1\mu)\,D(\mu\bar{\sigma}_1\xi_1)\,, \tag{4.2}$$

respectively, as shown in Fig. 8. Again, the number of elements in the extended CTMs are the same as the original ones. In this way we have reduced the double row system in Fig. 6 as single row one constructed from A', B, C, D', P_i, and S'_i. The spin fixing procedure from the left to right explained in the previous section is now applicable to the second row of spins $\{\tau\}$. It is straight forward to repeat the extension of HRTMs and CTMs to the vertical direction for $M-1$ times, we finally obtain the snapshot of the size $N\times M$ in the infinite system.

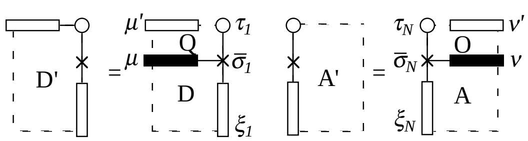

Fig. 8. Area extension of CTMs D and A.

§5. Conclusion and Discussion

We have explained the way of obtaining spin snapshot in the area of $N\times M$ for the 2D Ising model. The snapshot observation can be applied to various 2D lattice models with short range interaction, such as the IRF and the vertex models.[9] It is also possible to treat half-infinite or finite size systems and observe snapshot near the system boundary if we admit position dependence to HRTMs. (The finite system DMRG may be more appropriate than CTMRG in such a position dependent case.)

The calculations of conditional probability requires renormalized CTM and HRTM, that are converged to the infinite system size limit in the numerical algorithm of CTMRG. The convergence is quite slow near the critical temperature, and it is necessary to accelerate it. The same problem exists in the infinite system DMRG algorithm, and the problem has not been solved yet.

It is possible to apply the conventional real space renormalization group transformation, such as the majority rule for blocks of spins, to the obtained snapshots and calculate the critical indices. This suggests that both CTM and HRTM implicitly have information about criticality such as critical indices and scaling functions. To pull out these directly from CTM and HRTM, without looking at the snapshot is one of the future problem.

We finally comment about a relation between 2D classical systems and 1D quantum systems. The snapshot in the former corresponds to many time observation result in the latter. A snapshot can be regarded as a representative path in the path integral formulation of quantum systems. Successive observations in time-dependent DMRG[10,11] for numbers of time slices is the same type of computation.

1) K. Binder, "Monte Carlo Simulation in Statistical Physics: An Introduction", Springer Series in Solid-State Sciences **80** (Springer Berlin, 2002).
2) S. R. White: Phys. Rev. Lett. 69 (1992) 2863; Phys. Rev. B48 (1993) 10345.
3) M. Fannes, B. Nachtergale and R. F. Werner: Europhys. Lett. **10**, (1989) 633; M. Fannes, B. Nachtergale and R. F. Werner: Commun. Math. Phys. **144**, (1992) 443; M. Fannes, B. Nachtergale and R. F. Werner: Commun. Math. Phys. **174**, (1995) 477.
4) "Density-Matrix Renormalization", Springer Lecture Note in Physics 528, eds. I. Peschel, X. Wang, M. Kaulke and K. Hallberg, (Springer Berlin, 1999).
5) R.J. Baxter, J. Math. Phys. **9** (1968), 650; J. Stat. Phys. **19** (1978), 461; *Exactly Solved Models in Statistical Mechanics* (AcademicPress, London, 1982), p.363.
6) T. Nishino: J. Phys. Soc. Jpn. **64** (1995) 3598.
7) T. Nishino and K. Okunishi, J. Phys. Soc. Jpn. **65** (1996) 891; J. Phys. Soc. Jpn. **66**(1997) 3040.
8) We have represented the Ising model as the special parameter case of the IRF model.
9) A new critical point of a subset of symmetric 16-vertex model is reported in R. Otani, Thesis (Kobe University, 2002).
10) A.J. Daley, C. Kollath, U. Schollwöck, and G. Vidal: J. Stat. Mech. Theor. Exp. (2004) P04005.
11) S.R. White, and A.E. Feiguin, cond-mat/0403310.